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# CESIUM ION-NEUTRAL SCATTERING AND ION MOBILITY IN THE LOW FIELD LIMIT



by John W. Sheldon
Lewis Research Center
Cleveland, Ohio

TECHNICAL PREPRINT prepared for Thermionic Conversion Specialist Conference sponsored by the Institute of Electrical and Electronics Engineers
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by John Sheldon

Lewis Research Center
National Aeronautics and Space Administration
Cleveland, Ohio

32437

## Abstract

A semiclassical theory of cesium ion-neutral scattering with charge exchange is presented. The differential scattering cross section is presented and integrated to obtain total cross section and momentum-transfer cross section. The total cross section calculation gives good agreement with experiment. The momentum-transfer cross section, when compared in terms of ion mobility in the low field limit, also gives good agreement with experiment.

Author

## Introduction

Solutions to thermal plasma transport problems, such as those that arise in thermionics, require values for the energy-dependent differential cross sections of the various possible particle interactions. Integrals of the form

$$2\pi \int_0^\pi g(\theta)\sigma(\epsilon,\theta) \sin \theta \, d\theta$$

must be evaluated where $\sigma(\epsilon,\theta)$ is the differential cross section, $\epsilon$ is the relative energy of collision, $\theta$ is the scattering angle in the center of mass, and $g(\theta)$ is dictated by transport theory.

This paper is a presentation of a calculation of $\sigma(\epsilon,\theta)$ for the interaction of cesium ions with neutral atoms and the subsequent integration of the above integral for $g(\theta) = 1$ and $g(\theta) = 1 - \cos \theta$. The first case gives the total scattering cross section, the second, the momentum-transfer cross section; the latter is required to obtain the ion mobility in the low field limit. Since $\sigma(\epsilon,\theta)$ has not been determined experimentally, a comparison with experiment can only be made in terms of total scattering cross section and ion mobility. This comparison will illustrate the relation of beam measurements (total cross section) to ion mobility.

## Charge-Exchange Phenomena

A cesium ion moving past a cesium atom may exchange charge, the outermost electron making a transition from the ground state of one ion core to the other. The results of a calculation[1] of this transition probability are presented in figure 1. The minimum atomic separation during a collision, R, has an upper limit, $R_c$, beyond which the charge exchange probability, $P_o$, rapidly drops to zero. The energy dependence of $R_c$ is given by

$$R_c = \left(\frac{2}{\pi}\right)^{\frac{1}{2}} (A - B \ln \epsilon)$$

where A and B are constants dependent on atomic structure. The exchange probability may be approximated[2] by

$$P_o = 1/2 \quad \text{when} \quad R \leq R_c \qquad\qquad P_o = 0 \quad \text{when} \quad R > R_c \tag{1}$$

## Polarization Effect

If there were no deflection of the ion path past the atom, the total charge-exchange cross section $\sigma_x(\epsilon)$ would obviously be given by

$$\sigma_x(\epsilon) = (A - B \ln \epsilon)^2 \tag{2}$$

This energy dependence is indeed found at collision energies greater than a few electron volts; however, at lower collision energy the ion path is curved significantly toward the atom because of the interaction of the ionic field with the induced atomic multipoles. The leading term in the cesium multipole expansion is the dipole[2], which gives

$$U_{(r)} = -\frac{V}{r^4} \tag{3}$$

for the interaction potential $U_{(r)}$ where $r$ is the distance between the ion and the atom ($V = e^2\alpha/2$ where $e$ is the electron charge and $\alpha$ is the atomic polarizability). The relation between impact parameter, b, and distance of closest approach, R, is given by

$$\frac{b}{R} = \sqrt{1 + \frac{2V}{\epsilon R^4}} \tag{4}$$

for the monopole-dipole interaction. The generalized differential scattering cross section, $\sigma(\epsilon,\theta)$, computed[3] by classical methods for the polarization interaction potential is presented in figure 2. The scattering angle $\theta$ is in the center of mass system.

Semiclassical Differential Scattering Cross Section for Charge-Exchange and Elastic Scattering

Equations (1) and (4) may be combined[3,4] with the integrated orbit equation and the classical polarization cross section of figure 2 to give the differential charge-exchange cross section, $\sigma_x(\epsilon,\theta)$, and the differential elastic scattering cross section, $\sigma_e(\epsilon,\theta)$, as follows:

$$\sigma_x(\epsilon,\theta) = P_o\sigma(\epsilon,\pi - \theta) \tag{5}$$

$$\sigma_e(\epsilon,\theta) = (1 - P_o)\sigma(\epsilon,\theta) \tag{6}$$

In equations (5) and (6), $\theta$ is the apparent scattering angle in the center of mass system. The change in angular dependence from $\theta$ to $\pi - \theta$ is required in equation (5), since the particle identities as ion and atom reverse during the charge-exchange interaction.

The differential charge-exchange cross section and the differential elastic scattering cross section are presented in figure 3. The peak on the right side of the figure is due to charge exchange. The peak of infinite height on the left is a result of the classical approximation. A more exact treatment should yield a limited value of cross section for zero angle. The minimum angle for which the classical approximation is valid, $\theta^*$, is presented in figure 4; it is determined from uncertainty considerations.

## Total Scattering Cross Section

The total scattering cross section with charge exchange could be obtained by determining the area under a curve of the type shown in figure 3. Since the differential scattering cross section increases without limit as $\theta$ approaches zero, the area must be determined as a function of $\theta_m$, an arbitrarily chosen lower limit to the scattering angle. In practice, $\theta_m$ is determined by the minimum detectable scattering angle in a beam scattering apparatus. The total scattering cross section observed in this apparatus would be

$$\sigma_T(\epsilon,\theta_m) = 2\pi \int_{\theta_m}^{\pi} \sigma_e(\epsilon,\theta)\sin\theta\,d\theta + 2\pi \int_{\theta_m}^{\pi-\theta_c} \sigma_x(\epsilon,\theta)\sin\theta\,d\theta$$

If we require $\theta_m < \theta_c$, where $\theta_c$ is the smallest scattering angle at which the ion and atom at their point of closest approach are within the critical radius for charge exchange, the total scattering cross section reduces to the simple form[3]

$$\sigma_T(\epsilon,\theta_m) \cong \sqrt{\frac{3\pi e^2\alpha}{4\epsilon\theta_m}} \tag{7}$$

By referring to figure 4, we see the region where $\theta_m$ is larger than the quantum limit, $\theta^*$, but less than the critical angle for the onset of charge exchange to be the region of applicability of equation (7).

## Diffusion Cross Section and Mobility

The quantity most often needed for charge transport calculations is the diffusion cross section $\sigma_d(\epsilon)$, sometimes called the momentum-transfer cross section, which may be expressed as

$$\sigma_d(\epsilon) = 2\pi\int_0^\pi \sigma_e(\epsilon,\theta)(1 - \cos\theta)\sin\theta\, d\theta + 2\pi\int_0^\pi \sigma_x(\epsilon,\theta)(1 - \cos\theta)\sin\theta\, d\theta \tag{8}$$

Symmetry considerations in the above integrals yield

$$\sigma_d(\epsilon) \cong 2\sigma_x(\epsilon) \tag{9}$$

or, for low energy, we may use equation (4) to obtain[5]

$$\sigma_d(\epsilon) = 2\sigma_x(\epsilon)\left[1 + \frac{e^2\alpha}{\epsilon\sigma_x(\epsilon)^2}\left(\frac{\pi}{2}\right)^2\right] \tag{10}$$

The expression for ion mobility, $\mu$, in its own gas[2] is

$$\mu = \frac{3\sqrt{\pi}}{8}\frac{e}{\sqrt{mkT}\,N\overline{Q}} \tag{11}$$

where $m$ is atomic mass, $kT$ is vapor thermal energy, $N$ is vapor particle density, and $\overline{Q}$ is the following average of $\sigma_d(\epsilon)$:

$$\overline{Q} = \frac{1}{2(kT)^3}\int_0^\infty \epsilon^2\sigma_d(\epsilon)e^{-\frac{\epsilon}{kT}}\,d\epsilon \tag{12}$$

Inserting equation (10) in equation (12) and performing an approximate integration[6] gives

$$\overline{Q} \cong 2A^2 - 4AB\left(\frac{3}{2} - \mathcal{E} + \ln kT\right) + B^2\left[4\left(\frac{3}{2} - \mathcal{E}\right)\ln kT + 2(\ln kT)^2 + \mathcal{K}\right] + \left(\frac{\pi}{2}\right)^2\frac{e^2\alpha}{B^2kT\left(\frac{A}{B} - \ln kT\right)^2} \tag{13}$$

where $\mathcal{E}$ and $\mathcal{K}$ are the numerical constants 0.577 ..... and 2.492 ....., respectively.

## Comparison with Experiment

The total cross section expressed by equation (7) is compared with the UAC experiments[7] in figure 5. The angular resolution, a sensitive parameter in equation (7), is difficult to evaluate, and this can effect the location of the curve with respect to the ordinate. The experimental energy dependence of the data appear to confirm the theoretical prediction of $\epsilon^{-\frac{1}{2}}$.

Equations (11) and (13) give a value[6] of 0.07 ±0.03 $cm^2$/v-sec for the cesium ion mobility in cesium vapor compared with the 0.075 $cm^2$v-sec measured by Chanin and Steen[8] and 0.065 $cm^2$/v-sec measured by Dandurand and Holt[9]. The variation in the calculated value is the result of spread in the various sets of charge-exchange data[5].

## Concluding Remarks

A detailed presentation of the collision and mobility theory outlined in this paper are available elsewhere[3,6]. The purpose of this review has been to relate beam measurements of total scattering cross section[7] and total charge-exchange cross section[5] to each other and to ion mobility. The mobility discussed here is for the low field limit at which the thermal energy of the ions is greater than the energy they gain from the applied electric field between collisions. Inference that this is a suitable mobility for use in any particular thermionic diode problem is not intended.

REFERENCES

1. Demkov, Yu. N.: Quantum Mechanical Computations of Probability of Charge Exchange During Collisions. Sci. Memo. 146, Ser. Phys. Sci. 8, Leningrad State Univ., 1952, p. 74.

2. Holstein, T.: Mobilities of Positive Ions in Their Parent Gases. Jour. Phys. Chem., vol. 56, no. 7, Oct. 20, 1952, pp. 832-836.

3. Sheldon, J. W.: Semiclassical Calculation of the Differential Scattering Cross Section with Charge Exchange: Cesium Ions in Cesium Vapor. Ph.D. Thesis, Texas A. & M. Univ., Jan. 1964.

4. Mason, Edward A., and Vanderslice, Joseph T.: Elastic Scattering of Slow Ions in Gases. Jour. Chem. Phys., vol. 31, no. 3, Sept. 1959, pp. 594-600.

5. Sheldon, John W.: Mobilities of the Alkali Metal Ions in Their Own Vapor. Jour. Appl. Phys., vol. 34, no. 2, Feb. 1963, p. 444.

6. Sheldon, John W.: Mobility of Positive Ions in Their Own Gas: Determination of Average Momentum-Transfer Cross Section. NASA TN D-2408 (August 1964).

7. Bullis, R. H.: Low Energy Cesium Ion-Atom Collision Cross Section. IEEE Rep. on Thermionic Conversion Specialist Conf., Gatlingburg, Tenn., Oct. 7-9, 1963, pp. 1-9.

8. Chanin, Lorne M., and Steen, R. D.: Mobilities of Cesium Ions in Cesium. Phys. Rev., vol. 132, no. 6, Dec. 15, 1963, pp. 2554-2557.

9. Dandurand, P., and Holt, R. B.: Electron Density and Light Intensity Decay in Cesium Afterglows. Phys. Rev., vol. 82, 278.(1951) no. 2, Apr. 15, 1951, pp. 278-279.

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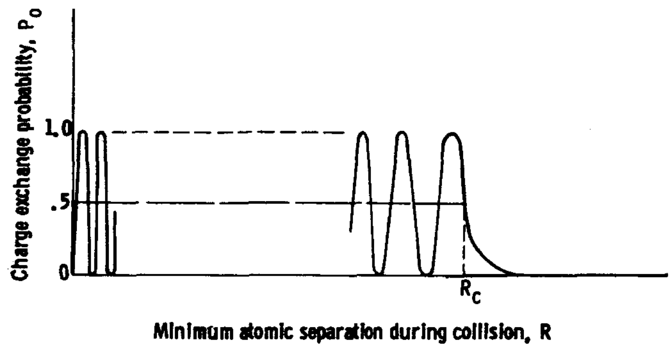


Figure 1. - Resonance charge-exchange probability.

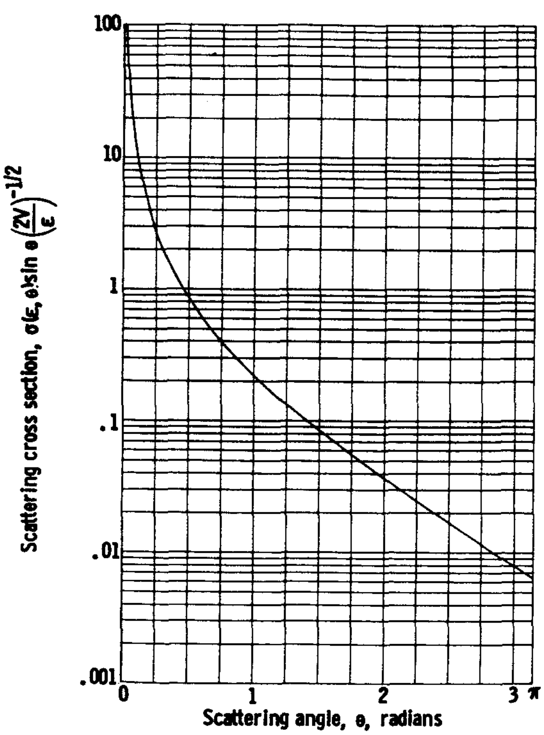


Figure 2. - Classical differential scattering cross section for polarization potential.

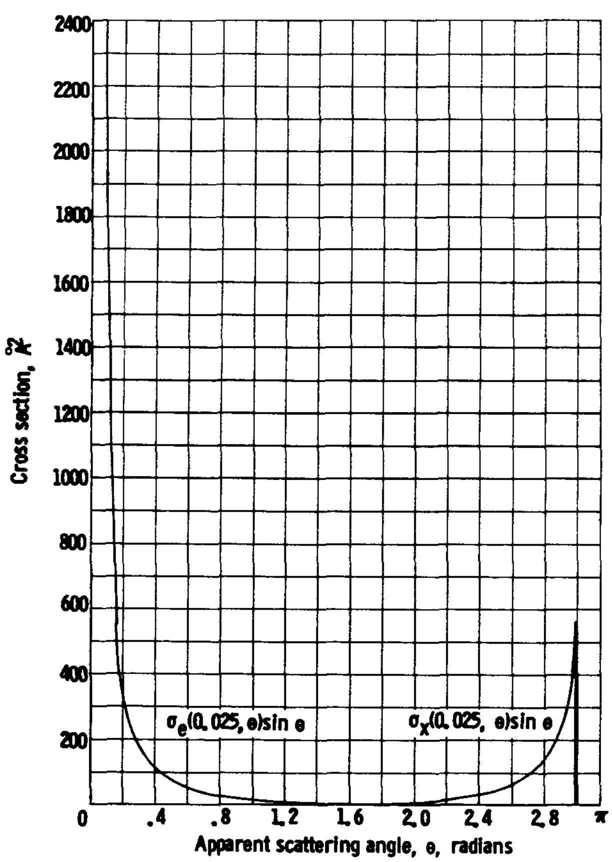


Figure 3. - Differential elastic scattering cross section and differential charge-exchange cross section for cesium ions in cesium vapor. Collision energy, 0.025 electron volt.

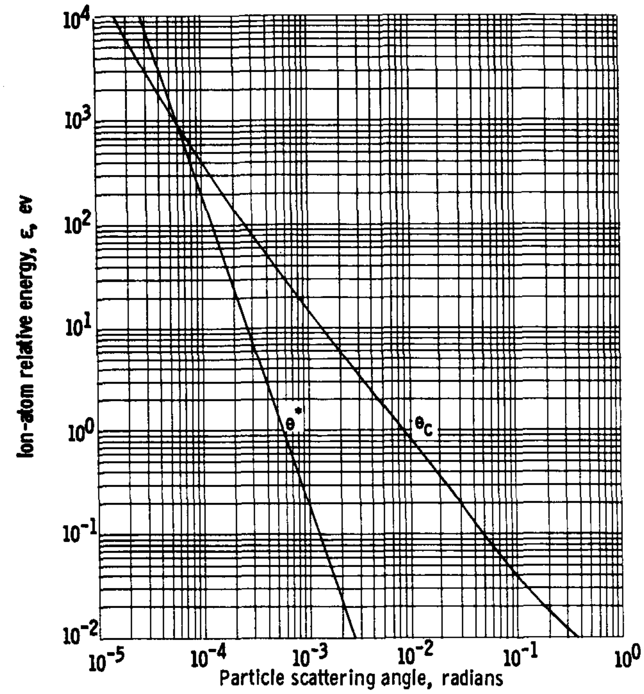


Figure 4. - Critical particle scattering angle $\theta_c$ and lower limit for valid classical calculation $\theta^*$ for cesium.

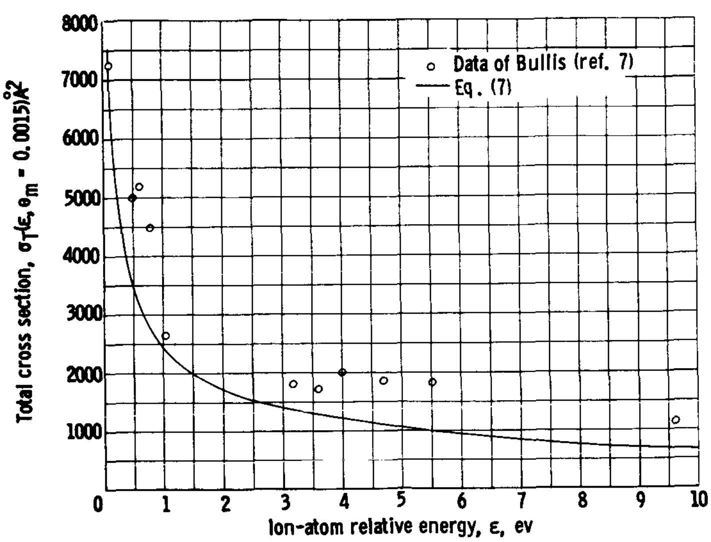


Figure 5. - The total scattering cross section for cesium ions in cesium vapor.